1 Synthesis and characterization of MeU(N[^{t}Bu]Ar)$_3$ 2

The solutions of IU(N[^{t}Bu]Ar)$_3$ (0.6000 g, 0.672 mmol and MeLi (0.53 mL of a 1.4 M diethyl ether solution, 0.739 mmol, 1.1 equiv) in diethyl ether (10 mL) were frozen. To the thawing solution of IU(N[^{t}Bu]Ar)$_3$ was added, by pipette, the thawing MeLi solution. The reaction mixture was allowed to warm to room temperature and stirred for 1h. After that time, the solution was filtered through Celite and the volatiles were removed under vacuum. The orange-brown solid was extracted with pentane, the resulting solution was filtered through Celite and the solvent was removed. The pentane extraction followed by filtration and solvent removal operations were repeated at least three more times until the presence of salts could no longer be detected on the Celite bed. The final solid was reextracted with pentane, the solution concentrated (2-3 mL) and stored at −35 °C. The yellow crystals collected after several days in two crops amounted to 0.315 g (60 % yield, 0.403 mmol). ^{1}H NMR (300 MHz, C_6D_6, 22°C): δ = 8.768 (s, 2H, *o*), 8.443 (s, 9H, *t-Bu*; possible overlap with a peak for 1H), 0.458 (s, 1H, *p*-Ar or *Me*), -3.468 (s, 6H, *Me*-Ar). Anal. calcd. for $C_{37}H_{57}N_3U$: C, 55.55; H, 7.18; N, 5.25. Found: C, 54.88; H, 7.18; N, 5.11.

2 Supporting information for ADF calculations

The calculations were carried out using the Amsterdam Density Functional (ADF) package.[1,2,3]

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 *   Amsterdam Density Functional  (ADF)         2000.02   17 July, 2000
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*
 *   Online information and documentation:  http://www.scm.com
*
 *   E-mail:  support@scm.com   info@scm.com
```

The input file for the calculation $(H_2N)_3USiH_3$ is given below. Other input files are similar to this and are not shown.

```
$ADFBIN/dirac < $ADFRESOURCES/Dirac/U
$ADFBIN/dirac < $ADFRESOURCES/Dirac/N
```

```
$ADFBIN/dirac < $ADFRESOURCES/Dirac/H
$ADFBIN/dirac < $ADFRESOURCES/Dirac/Si

$ADFBIN/adf << eor
CREATE U $ADFRESOURCES/ZORA/V/U
xc
GGA pw91
end
relativistic zora
corepotentials TAPE12 &
U 1
end
end input
eor
mv TAPE21 t21.U

$ADFBIN/adf << eor
CREATE N $ADFRESOURCES/ZORA/V/N
xc
GGA pw91
end
relativistic zora
corepotentials TAPE12 &
N 2
end
end input
eor
mv TAPE21 t21.N

$ADFBIN/adf << eor
CREATE H $ADFRESOURCES/ZORA/V/H
xc
GGA pw91
end
relativistic zora
corepotentials TAPE12 &
H 3
end
end input
eor
mv TAPE21 t21.H

$ADFBIN/adf << eor
CREATE Si $ADFRESOURCES/ZORA/V/Si
xc
```

```
GGA pw91
end
relativistic zora
corepotentials TAPE12 &
Si 4
end
end input
eor
mv TAPE21 t21.Si


$ADFBIN/adf << eor > siU.out
title uranium silyl - zora relativistic - spin unrestricted

atoms Z-matrix
1 XX 0 0 0 0 0 0
2 U 1 0 0 1.0 0 0
3 N 2 1 0 2.230 110 0
4 N 2 1 3 2.230 110 120
5 N 2 1 3 2.230 110 240
6 H 3 2 1 1.015 120 0
7 H 3 2 1 1.015 120 180
8 H 4 2 1 1.015 120 0
9 H 4 2 1 1.015 120 180
10 H 5 2 1 1.015 120 0
11 H 5 2 1 1.015 120 180
12 Si 2 3 6 d 110 0
13 H 12 2 3 1.484 110 180
14 H 12 2 3 1.484 110 60
15 H 12 2 3 1.484 110 300
end

geovar
d 2.950
end

Symmetry=C(3v)

fragments
U t21.U
N t21.N
H t21.H
Si t21.Si
end
```

```
xc
gga pw91
end


relativistic zora

unrestricted

charge 0 2

corepotentials TAPE12 &
U 1
N 2
H 3
Si 4
end
scf
ITERATIONS 99
MIXING 0.05
end

geometry
optim selected internal
converge Rad=0.005
step Rad=0.002
end


end input

eor

adfrom_ADF1999_pentiumlinux TAPE21

mv logfile meU.log

rm -f [A-Z]* t*
```

Table S1. Calculated[a] Covalent Radii (r_E) for Group 14 Elements[b]

	r_E	$d_{E\text{-}H}$	$r_E - d_{E\text{-}H}$[c]	$\lvert\delta_E^+ - \delta_H^-\rvert$[d]
C_2H_6	0.770	1.092	0.322	0.145
Si_2H_6	1.178	1.484	0.306	0.273
Ge_2H_6	1.215	1.528	0.313	0.244
Sn_2H_6	1.392	1.710	0.318	0.351

[a]See text for computational details; distances given in Å.
[b]E = C, Si, Ge, and Sn.
[c]This quantity should approximate r_H for highly covalent compounds.
[d]Measure of the bond ionicity from calculated Hirshfeld charge differences.

3 Supporting information for X-ray crystal structures

3.1 General considerations

The X-ray data collections were carried out on a Siemens Platform three-circle goniometer with a CCD detector using Mo-Kα radiation (λ = 0.71073 Å). The data were processed utilizing the program SAINT supplied by Siemens Industrial Automation, Inc.

3.2 X-ray crystal structure of $(Me_3Si)_3SiU(N[^tBu]Ar)_3$ (1)

Inside the glove-box, crystals of **1** grown from a concentrated diethyl ether solution at −35 °C were coated with Paratone N oil (an Exxon product) on a microscope slide. A red plate of approximate dimensions 0.23 x 0.12 x 0.10 mm^3 was selected and mounted with wax on a glass fiber. A total of 13514 reflections ($-17 \le h \le 15$, $-15 \le k \le 17$, $-16 \le l \le 16$) were collected at 183(2) K in the θ range of 2.00 to 23.28 °, of which 8079 were unique (R_{int} = 0.0355). The structure was solved by direct methods (SHELXTL V5.1, G. M. Sheldrick and Siemens Industrial Automation, Inc., 1997) in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically and hydrogen atoms were placed in calculated (d_{CH} = 0.96 Å) positions. The residual peak and hole electron density were 1.259 and −0.430 e·Å^{-3}, respectively, and are in the typical range due to the scattering effect of the large uranium nucleus. A semi-empirical absorption correction was applied based on pseudo-psi-scans with maximum and minimum transmissions equal to 0.7840 and 0.5907, respectively. The least squares refinement converged normally with residuals of R_1=0.0366, wR_2=0.1240 based on $I > 2\sigma I$ and GOF = 1.175 (based on F^2). No extinction coefficient was applied to the refinement.

Crystal and refinement data: formula = $C_{45}H_{81}N_3Si_4U$, space group $P\bar{3}$, a = 15.8914(5) Å, b = 15.8914(5) Å, c = 15.0757 Å, α = 90 °, β = 90 °, γ = 120 °, Z = 2, V = 3297.1(2) Å^3, D_{calcd} = 1.022 g·cm^{-3}, $F(000)$ = 1040, R (based on F) = 0.0420, wR (based on F^2) = 0.1267.

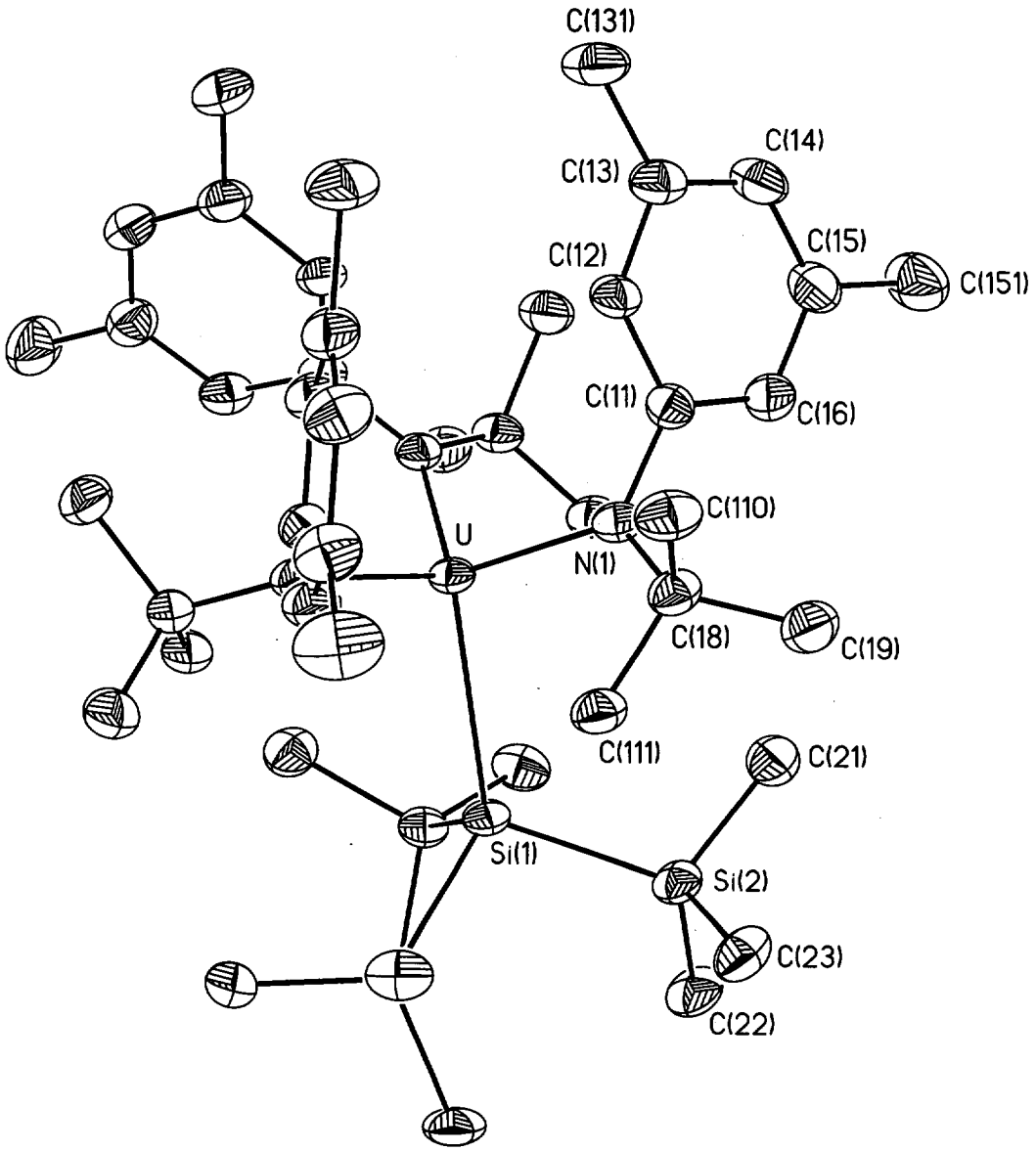

Figure 1: Structural representation of compound **1** with thermal ellipsoids at the 35% probability level.

Table S2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å^2 x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
U	6667	3333	2017(1)	35(1)
Si(1)	6667	3333	-33(2)	39(1)
Si(2)	5142(1)	2354(1)	-704(1)	46(1)
N(1)	5163(4)	2742(4)	2504(3)	39(1)
C(11)	4787(4)	1990(5)	3167(4)	41(2)
C(14)	4163(5)	531(5)	4439(5)	56(2)
C(23)	4370(6)	2946(6)	-732(5)	59(2)
C(18)	4542(5)	3172(5)	2292(4)	45(2)
C(13)	4828(5)	1486(5)	4683(4)	51(2)
C(22)	5218(6)	2017(6)	-1898(4)	63(2)
C(12)	5119(5)	2200(5)	4038(4)	43(2)
C(16)	4128(5)	1019(5)	2954(4)	49(2)
C(15)	3809(5)	289(5)	3580(5)	56(2)
C(131)	5209(6)	1732(6)	5609(4)	65(2)
C(111)	5102(5)	3980(5)	1625(4)	48(2)
C(19)	3566(5)	2438(6)	1898(5)	56(2)
C(21)	4429(6)	1174(5)	-90(5)	62(2)
C(110)	4364(6)	3615(6)	3129(4)	56(2)
C(151)	3101(7)	-748(6)	3335(6)	79(3)

Table S3. Bond lengths [Å] and angles [°] for 1.

U-N(1)#1	2.210(5)
U-N(1)#2	2.210(5)
U-N(1)	2.210(5)
U-Si(1)	3.091(3)
Si(1)-Si(2)#1	2.354(2)
Si(1)-Si(2)	2.354(2)
Si(1)-Si(2)#2	2.354(2)
Si(2)-C(21)	1.879(7)
Si(2)-C(23)	1.884(7)
Si(2)-C(22)	1.899(7)
N(1)-C(11)	1.439(8)
N(1)-C(18)	1.490(8)
C(11)-C(12)	1.392(9)
C(11)-C(16)	1.401(9)
C(14)-C(15)	1.387(10)
C(14)-C(13)	1.397(10)
C(18)-C(111)	1.519(9)
C(18)-C(19)	1.520(9)
C(18)-C(110)	1.538(9)
C(13)-C(12)	1.386(9)
C(13)-C(131)	1.495(10)
C(16)-C(15)	1.381(10)
C(15)-C(151)	1.505(11)
N(1)#1-U-N(1)#2	109.56(12)
N(1)#1-U-N(1)	109.56(12)
N(1)#2-U-N(1)	109.56(12)
N(1)#1-U-Si(1)	109.38(12)
N(1)#2-U-Si(1)	109.38(12)
N(1)-U-Si(1)	109.38(12)
Si(2)#1-Si(1)-Si(2)	102.91(9)
Si(2)#1-Si(1)-Si(2)#2	102.91(9)
Si(2)-Si(1)-Si(2)#2	102.91(9)
Si(2)#1-Si(1)-U	115.43(8)
Si(2)-Si(1)-U	115.43(8)
Si(2)#2-Si(1)-U	115.43(8)
C(21)-Si(2)-C(23)	107.0(4)
C(21)-Si(2)-C(22)	106.1(4)
C(23)-Si(2)-C(22)	105.6(3)
C(21)-Si(2)-Si(1)	110.9(2)
C(23)-Si(2)-Si(1)	113.0(2)

C(22)-Si(2)-Si(1)	113.8(3)
C(11)-N(1)-C(18)	115.8(5)
C(11)-N(1)-U	119.7(4)
C(18)-N(1)-U	123.9(4)
C(12)-C(11)-C(16)	117.7(6)
C(12)-C(11)-N(1)	120.4(6)
C(16)-C(11)-N(1)	121.7(6)
C(15)-C(14)-C(13)	121.9(6)
N(1)-C(18)-C(111)	106.7(5)
N(1)-C(18)-C(19)	112.8(6)
C(111)-C(18)-C(19)	109.4(5)
N(1)-C(18)-C(110)	110.4(5)
C(111)-C(18)-C(110)	108.7(6)
C(19)-C(18)-C(110)	108.7(6)
C(12)-C(13)-C(14)	117.8(6)
C(12)-C(13)-C(131)	121.0(7)
C(14)-C(13)-C(131)	121.2(6)
C(13)-C(12)-C(11)	122.3(6)
C(15)-C(16)-C(11)	121.8(6)
C(16)-C(15)-C(14)	118.5(7)
C(16)-C(15)-C(151)	120.8(7)
C(14)-C(15)-C(151)	120.7(7)

Symmetry transformations used to generate equivalent atoms: #1 -y+1, x-y, z #2 -x+y+1, -x+1, z

Table S4. Anisotropic displacement parameters [Å^2 x 10^3] for 1.

	U11	U22	U33	U23	U13	U12
U	42(1)	42(1)	21(1)	0	0	21(1)
Si(1)	48(1)	48(1)	22(1)	0	0	24(1)
Si(2)	53(1)	54(1)	29(1)	-7(1)	-6(1)	26(1)
N(1)	48(3)	45(3)	26(3)	-2(2)	-1(2)	25(3)
C(11)	41(4)	49(4)	32(3)	0(3)	5(3)	23(3)
C(14)	65(5)	53(4)	41(4)	10(3)	12(3)	24(4)
C(23)	59(5)	81(5)	45(4)	-11(4)	-11(3)	41(4)
C(18)	47(4)	59(4)	33(3)	-3(3)	-2(3)	31(3)
C(13)	60(4)	62(5)	35(4)	5(3)	6(3)	34(4)
C(22)	74(5)	80(5)	32(4)	-15(4)	-13(4)	36(4)
C(12)	48(4)	49(4)	30(3)	1(3)	6(3)	22(3)
C(16)	49(4)	58(4)	33(3)	-3(3)	0(3)	23(4)
C(15)	57(4)	49(4)	49(4)	3(3)	8(3)	18(4)
C(131)	88(6)	74(5)	32(4)	7(4)	1(4)	40(5)
C(111)	54(4)	59(4)	33(4)	1(3)	-3(3)	30(4)
C(19)	56(4)	71(5)	44(4)	1(4)	-4(3)	34(4)
C(21)	65(5)	59(5)	47(4)	-4(4)	-6(4)	21(4)
C(110)	71(5)	72(5)	39(4)	-2(3)	2(3)	47(4)
C(151)	90(6)	54(5)	66(6)	2(4)	1(5)	15(5)

3.3 X-ray crystal structure of MeU(N[^{t}Bu]Ar)$_3$ (2)

Inside the glove-box, crystals of **2** grown from a concentrated pentane solution at −35 °C were coated with Paratone N oil (an Exxon product) on a microscope slide. An orange yellow plate of approximate dimensions 0.38 x 0.16 x 0.11 mm^3 was selected and mounted with wax on a glass fiber. A total of 7233 reflections ($-10 \leq h \leq 9$, $-12 \leq k \leq 12$, $-15 \leq l \leq 18$) were collected at 183(2) K in the θ range of 2.50 to 23.29 °, of which 5095 were unique ($R_{int} = 0.0497$). The structure was solved using the Patterson method (SHELXTL V5.1, G. M. Sheldrick and Siemens Industrial Automation, Inc., 1997) in conjunction with standard difference Fourier techniques. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were found in the electronic density map with the exception of H11C, H15C, H13A, H13B, H13C, H23A, H23B, H23C which were placed in calculated ($d_{CH} = 0.96$ Å) positions. The residual peak and hole electron density were 1.733 and −1.744 e·Å^{-3}, respectively, and are in the typical range due to the scattering effect of the large uranium nucleus. A semi-empirical absorption correction was applied based on pseudo-psi-scans with maximum and minimum transmissions equal to 0.6375 and 0.2798, respectively. The least squares refinement converged normally with residuals of R_1=0.0334, wR_2=0.0859 based on $I > 2\sigma I$ and GOF = 1.076 (based on F^2). No extinction coefficient was applied to the refinement.

Crystal and refinement data: formula = $C_{37}H_{56}N_3U$, space group $P\bar{1}$, a = 9.6053(17) Å, b = 11.572(2) Å, c = 16.567(3) Å, α = 80.534(3) °, β = 88.108(3) °, γ = 89.743(3) °, Z = 2, V = 1815.4(6) Å^3, D_{calcd} = 1.429 g·cm^{-3}, $F(000)$ = 782, R (based on F) = 0.0350, wR (based on F^2) = 0.0872.

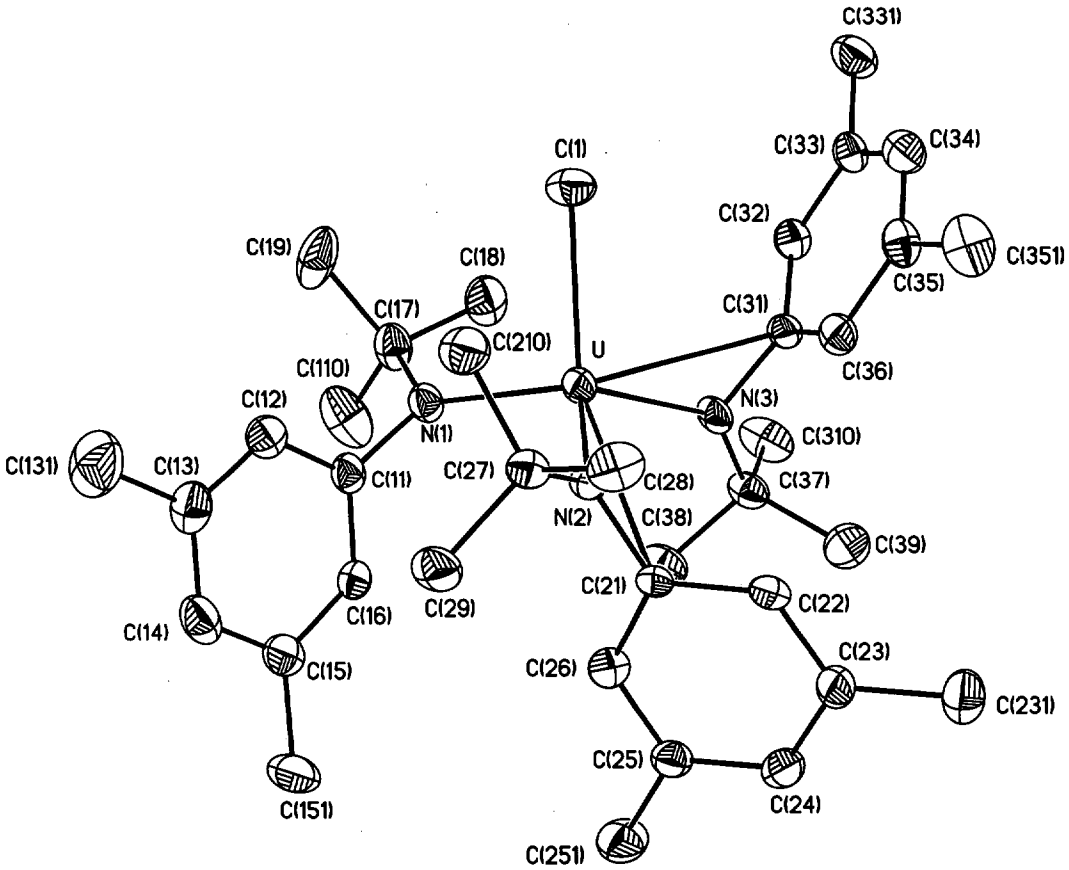

Figure 2: Structural representation of compound **2** with thermal ellipsoids at the 35% probability level.

Table S5. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [Å^2 x 10^3] for 2. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
U	1748(1)	2158(1)	2755(1)	28(1)
N(1)	2559(5)	2318(4)	3965(3)	35(1)
C(1)	-700(7)	1771(6)	3159(5)	46(2)
N(2)	1913(4)	3832(4)	1864(3)	30(1)
N(3)	2594(5)	613(4)	2253(3)	34(1)
C(11)	3144(6)	3450(5)	4029(3)	35(1)
C(12)	2337(7)	4336(5)	4287(3)	39(1)
C(13)	2859(7)	5439(6)	4291(4)	48(2)
C(14)	4241(8)	5676(6)	4033(4)	48(2)
C(15)	5065(7)	4823(6)	3771(4)	44(2)
C(16)	4507(6)	3713(6)	3776(3)	36(1)
C(17)	2473(7)	1445(5)	4729(4)	46(2)
C(19)	1293(12)	1756(8)	5306(5)	73(3)
C(21)	3035(5)	3768(4)	1292(3)	28(1)
C(22)	2832(6)	3558(5)	498(3)	30(1)
C(23)	3941(6)	3384(5)	-30(4)	37(1)
C(24)	5283(6)	3434(5)	247(4)	38(1)
C(25)	5539(5)	3645(5)	1031(3)	35(1)
C(26)	4402(5)	3835(5)	1536(3)	32(1)
C(27)	1190(6)	4960(5)	1837(4)	34(1)
C(29)	2197(8)	5912(6)	2016(5)	46(2)
C(31)	1347(5)	218(5)	1928(3)	31(1)
C(32)	581(6)	-745(5)	2336(4)	37(1)
C(33)	-718(6)	-996(5)	2061(4)	40(1)
C(34)	-1252(6)	-289(6)	1387(4)	43(1)
C(35)	-521(6)	660(5)	966(4)	40(1)
C(36)	782(7)	903(5)	1253(4)	37(1)
C(37)	3934(6)	53(5)	2108(4)	38(1)
C(39)	4254(8)	162(8)	1186(5)	58(2)
C(110)	3829(13)	1353(9)	5166(7)	76(3)
C(18)	2118(9)	282(7)	4486(5)	56(2)
C(131)	1923(10)	6412(7)	4536(6)	79(2)
C(151)	6543(9)	5084(9)	3484(5)	70(3)
C(210)	65(9)	4730(9)	2510(6)	48(2)
C(28)	527(7)	5362(6)	1015(4)	44(2)
C(231)	3706(7)	3115(7)	-865(4)	53(2)

C(251)	6999(7)	3674(8)	1328(6)	57(2)
C(310)	3939(8)	-1244(6)	2510(6)	59(2)
C(38)	5037(7)	706(7)	2489(6)	51(2)
C(331)	-1554(8)	-2011(7)	2518(5)	52(2)
C(351)	-1109(9)	1407(7)	220(5)	57(2)

Table S6. Bond lengths [Å] and angles [°] for 2.

U-N(1)	2.211(4)
U-N(3)	2.231(4)
U-N(2)	2.237(4)
U-C(1)	2.446(7)
U-C(31)	2.849(5)
U-C(21)	3.035(5)
N(1)-C(11)	1.449(7)
N(1)-C(17)	1.484(8)
N(2)-C(21)	1.422(7)
N(2)-C(27)	1.470(7)
N(3)-C(31)	1.436(7)
N(3)-C(37)	1.469(8)
C(11)-C(16)	1.381(8)
C(11)-C(12)	1.396(9)
C(12)-C(13)	1.374(9)
C(13)-C(14)	1.396(10)
C(13)-C(131)	1.536(10)
C(14)-C(15)	1.378(10)
C(15)-C(16)	1.392(9)
C(15)-C(151)	1.498(10)
C(17)-C(110)	1.507(12)
C(17)-C(18)	1.509(10)
C(17)-C(19)	1.538(11)
C(21)-C(26)	1.393(7)
C(21)-C(22)	1.397(8)
C(22)-C(23)	1.390(8)
C(23)-C(24)	1.387(9)
C(23)-C(231)	1.493(8)
C(24)-C(25)	1.391(8)
C(25)-C(26)	1.392(8)
C(25)-C(251)	1.503(9)
C(27)-C(210)	1.518(10)
C(27)-C(28)	1.524(9)
C(27)-C(29)	1.540(9)
C(31)-C(36)	1.385(9)
C(31)-C(32)	1.403(8)
C(32)-C(33)	1.390(8)
C(33)-C(34)	1.383(9)
C(33)-C(331)	1.508(10)
C(34)-C(35)	1.382(9)
C(35)-C(36)	1.399(9)
C(35)-C(351)	1.512(10)

C(37)-C(38)	1.517(9)
C(37)-C(39)	1.533(10)
C(37)-C(310)	1.539(9)
N(1)-U-N(3)	113.32(17)
N(1)-U-N(2)	112.61(16)
N(3)-U-N(2)	113.31(17)
N(1)-U-C(1)	99.0(2)
N(3)-U-C(1)	108.2(2)
N(2)-U-C(1)	109.3(2)
N(1)-U-C(31)	133.23(17)
N(3)-U-C(31)	29.79(16)
N(2)-U-C(31)	110.89(16)
C(1)-U-C(31)	82.0(2)
N(1)-U-C(21)	116.37(15)
N(3)-U-C(21)	89.59(16)
N(2)-U-C(21)	26.10(15)
C(1)-U-C(21)	130.2(2)
C(31)-U-C(21)	95.98(15)
C(11)-N(1)-C(17)	116.5(4)
C(11)-N(1)-U	115.4(3)
C(17)-N(1)-U	127.8(4)
C(21)-N(2)-C(27)	118.0(4)
C(21)-N(2)-U	110.1(3)
C(27)-N(2)-U	131.5(3)
C(31)-N(3)-C(37)	119.9(4)
C(31)-N(3)-U	99.7(3)
C(37)-N(3)-U	140.0(3)
C(16)-C(11)-C(12)	117.7(5)
C(16)-C(11)-N(1)	120.3(5)
C(12)-C(11)-N(1)	121.8(5)
C(13)-C(12)-C(11)	122.1(6)
C(12)-C(13)-C(14)	118.8(6)
C(12)-C(13)-C(131)	120.8(7)
C(14)-C(13)-C(131)	120.3(6)
C(15)-C(14)-C(13)	120.6(6)
C(14)-C(15)-C(16)	119.2(6)
C(14)-C(15)-C(151)	120.5(7)
C(16)-C(15)-C(151)	120.3(7)
C(11)-C(16)-C(15)	121.6(6)
N(1)-C(17)-C(110)	111.5(6)
N(1)-C(17)-C(18)	107.0(5)
C(110)-C(17)-C(18)	110.0(7)
N(1)-C(17)-C(19)	110.8(6)
C(110)-C(17)-C(19)	109.7(8)

C(18)-C(17)-C(19)	107.7(6)
C(26)-C(21)-C(22)	117.6(5)
C(26)-C(21)-N(2)	119.8(5)
C(22)-C(21)-N(2)	122.5(4)
C(26)-C(21)-U	101.0(3)
C(22)-C(21)-U	120.4(3)
N(2)-C(21)-U	43.8(2)
C(23)-C(22)-C(21)	121.9(5)
C(24)-C(23)-C(22)	118.4(5)
C(24)-C(23)-C(231)	120.3(5)
C(22)-C(23)-C(231)	121.3(5)
C(23)-C(24)-C(25)	121.9(5)
C(24)-C(25)-C(26)	118.0(5)
C(24)-C(25)-C(251)	121.3(6)
C(26)-C(25)-C(251)	120.7(6)
C(25)-C(26)-C(21)	122.1(5)
N(2)-C(27)-C(210)	104.7(6)
N(2)-C(27)-C(28)	112.1(5)
C(210)-C(27)-C(28)	109.8(6)
N(2)-C(27)-C(29)	110.7(5)
C(210)-C(27)-C(29)	110.0(6)
C(28)-C(27)-C(29)	109.4(5)
C(36)-C(31)-C(32)	118.6(5)
C(36)-C(31)-N(3)	118.7(5)
C(32)-C(31)-N(3)	122.1(5)
C(36)-C(31)-U	93.5(3)
C(32)-C(31)-U	118.3(4)
N(3)-C(31)-U	50.5(2)
C(33)-C(32)-C(31)	120.0(6)
C(34)-C(33)-C(32)	119.7(6)
C(34)-C(33)-C(331)	120.5(6)
C(32)-C(33)-C(331)	119.7(6)
C(35)-C(34)-C(33)	121.8(6)
C(34)-C(35)-C(36)	117.7(6)
C(34)-C(35)-C(351)	121.0(6)
C(36)-C(35)-C(351)	121.3(6)
C(31)-C(36)-C(35)	122.1(6)
N(3)-C(37)-C(38)	106.8(5)
N(3)-C(37)-C(39)	110.0(5)
C(38)-C(37)-C(39)	109.2(6)
N(3)-C(37)-C(310)	111.5(5)
C(38)-C(37)-C(310)	109.1(6)
C(39)-C(37)-C(310)	110.1(6)

Symmetry transformations used to generate equivalent atoms:

Table S7. Anisotropic displacement parameters [Å^2 x 10^3] for 2.

	U11	U22	U33	U23	U13	U12
U	31(1)	24(1)	30(1)	-5(1)	0(1)	-3(1)
N(1)	40(3)	35(3)	28(2)	-5(2)	-4(2)	-6(2)
C(1)	38(3)	44(4)	55(4)	-4(3)	7(3)	-6(3)
N(2)	27(2)	33(2)	29(2)	-5(2)	-1(2)	-4(2)
N(3)	37(2)	22(2)	46(3)	-13(2)	-2(2)	-4(2)
C(11)	43(3)	38(3)	24(3)	-6(2)	-5(2)	-4(3)
C(12)	45(3)	38(3)	31(3)	-2(2)	-2(3)	-3(3)
C(13)	67(4)	42(4)	37(3)	-9(3)	0(3)	3(3)
C(14)	71(4)	37(4)	35(3)	-4(3)	-5(3)	-17(3)
C(15)	50(4)	54(4)	28(3)	-3(3)	-5(3)	-13(3)
C(16)	41(3)	41(3)	26(3)	-10(3)	1(2)	-5(3)
C(17)	66(4)	34(3)	37(3)	-5(3)	-5(3)	-4(3)
C(19)	133(8)	46(5)	38(4)	-7(4)	29(5)	-9(5)
C(21)	28(3)	26(3)	29(3)	-3(2)	3(2)	-8(2)
C(22)	25(3)	30(3)	33(3)	-1(2)	-3(2)	-5(2)
C(23)	47(3)	31(3)	34(3)	-8(2)	3(3)	-9(2)
C(24)	38(3)	37(3)	38(3)	-6(3)	8(3)	-2(2)
C(25)	29(3)	41(3)	35(3)	-3(3)	-2(2)	-5(2)
C(26)	30(3)	34(3)	30(3)	2(2)	-5(2)	4(2)
C(27)	32(3)	33(3)	35(3)	-3(2)	0(2)	-3(2)
C(29)	47(4)	28(4)	63(4)	-10(3)	7(4)	-6(3)
C(31)	30(3)	27(3)	37(3)	-11(2)	3(2)	-3(2)
C(32)	40(3)	34(3)	38(3)	-9(3)	-3(3)	-1(3)
C(33)	42(3)	35(3)	46(3)	-20(3)	2(3)	-9(3)
C(34)	36(3)	41(4)	54(4)	-17(3)	-3(3)	3(3)
C(35)	45(3)	36(3)	40(3)	-13(3)	-8(3)	5(3)
C(36)	47(3)	26(3)	40(3)	-10(3)	3(3)	-6(3)
C(37)	35(3)	28(3)	53(4)	-9(3)	-4(3)	1(2)
C(39)	44(4)	68(5)	66(5)	-26(4)	7(3)	5(4)
C(110)	99(8)	49(5)	81(7)	-3(5)	-38(6)	-4(5)
C(18)	81(5)	49(4)	36(4)	-1(3)	0(4)	-12(4)
C(131)	101(6)	51(5)	88(6)	-23(4)	15(5)	10(4)
C(151)	65(5)	92(7)	51(4)	-10(4)	5(4)	-47(5)
C(210)	42(4)	39(5)	65(6)	-15(4)	6(3)	4(4)
C(28)	42(3)	41(4)	44(4)	7(3)	-1(3)	8(3)
C(231)	55(4)	67(5)	41(4)	-18(3)	-3(3)	-2(3)
C(251)	30(3)	84(6)	55(5)	-12(4)	-1(3)	-1(3)
C(310)	41(4)	35(4)	101(6)	-13(4)	-10(4)	7(3)

C(38)	38(4)	44(4)	70(6)	-8(4)	-8(4)	0(3)
C(331)	49(4)	53(4)	55(4)	-7(4)	-4(4)	-18(3)
C(351)	67(5)	43(4)	60(5)	-8(3)	-16(4)	8(4)

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